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ChemOffice Down Under

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Bill Suthers is a PhD student in chemistry at the University of Queensland, Australia. Within his research he synthesises structures, using detailed NMR work and theoretical calculations. He must also produce 3D pictures for presentation. Bill writes, "All this was eventually achieved with the software we had available, but the quality of output, and difficulty of use, meant that it was a long and trying process." Bill has turned to ChemOffice to increase his effectiveness and productivity.

As a Ph.D. student about to start writing my thesis I was most interested to see what ChemOffice Ultra had to offer. Our current chemical software worked--but was not very stable, had poor compatibility between programs, and often lacked outputs suitable for either presentation at conference or publication. Hopefully ChemOffice would be able to reduce my struggles over the coming months!

ChemDraw

I found ChemDraw to have an easy learning curve with intuitive tools that had me drawing structures within a couple of minutes. The ability to magnify and reduce the drawing with one mouse click made working with small and complex diagrams a snap, and working with an enlarged interface will make it easy on my eyes over a long period. The Online Help was well organized and enabled me to find out how to do more complex operations easily without needing to resort to hours sifting through the manual. Plenty of templates of both simple and more complex cyclic systems (and many others), again save time. Many simple things, like the quick interface to the "Align Objects" menu, combine to mean that you can be very productive, even if you've never used ChemDraw before! Complex groups of objects could be re-sized and retain their relative positions perfectly. The ability to save settings and configuration with the document, and move them between machines if necessary, was superb in our multiuser/multimachine environment. The settings themselves are very intelligently organized, such that with only about five parameters all the properties of the many drawing elements can be customized, thus greatly reducing the time necessary to personalize the output to my requirements.

Chem3D

To be able to simply paste the ChemDraw diagrams directly into Chem3D is a great time-saver and allows rapid shifting between the two programs. Running MM2 minimisations is a breeze, and the ability to watch the process graphically in real time is superb. Full details of the process are automatically provided as well. The trackball method of rotating the model allows extremely efficient viewing of the result, and the range of display formats meant I could always find a view that clearly represented the effects I was examining. In addition, it can be printed in full color for perfect presentation or publication.

If first impressions are any guide,
she'll be purchasing a copy of ChemInfo Pro ASAP.

ChemInfo

The ChemACX database is excellent! In designing synthetic schema, knowledge of which proposed intermediates are commercially available is priceless. Normally this requires lengthy naming of the compounds, and searching through catalogues to determine who, if anyone, sells it. Not with ChemACX! You don't even have to name your structure! Just drag the structure from ChemDraw into the structure window of ChemFinder and let it do the rest. In a flash you know if it's available, from whom, and in what quantity in addition to other useful data like CAS registry numbers. A fantastic timesaver! I was so impressed with it that I loaned it to our Purchasing Officer for the afternoon. If first impressions are any guide she'll be purchasing a copy of ChemInfo Pro ASAP.

ChemFinder

Never before having used a database access program such as ChemFinder, I was worried that I wouldn't be able to produce anything useful...Wrong! Half an hour with the manual, and I was not only accessing, but searching and getting useful data. For my field of Organic Synthesis, the ChemPrep and Chem-Select databases are superb. In my first two hours with the system, I had conducted reaction searches that turned up extremely interesting references, in journals commonly available, for reactions that my colleagues were struggling with that day. If I had had this sort of capability during my time at the bench, I can only think longingly about the time I would have saved looking up procedures.

My most dominant feeling at this point is, "I wish I had this earlier!" Much of my previous work would have been so much easier and quicker. And as to the writeup, well, it's not going to be painless, but ChemOffice will be making at least that part of it hassle free.

Footnote: This Article was first published in the CS Catalyst. Check it out at: http://www.camsoft.com

Comments

During 1-30 September 1998, all comments on this poster should be sent by e-mail to ecsoc@listserv.arizona.edu with e0005 as the message subject of your e-mail. After the conference, please send all the comments and reprints requests to the author.